

A stochastic approach to chaotic diffusion

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Abstract : The crucial question of instability of classical motion in Hamiltonian systems essentially rests on the curvature (or second derivative) of the potential. While the local linear stability analysis around the fixed points is based on assumption of constant curvature, we take full account of the time-dependence of this quantity in the chaotic regime by considering it to be a stochastic process, stochasticity being due to deterministic chaotic motion. Based on the theory of multiplicative noise we show that the correlation between the fluctuation of the curvature of the potential leads to chaotic diffusion. A rationalisation of the origin of the exponential divergence of initially nearby trajectories and also of the exponential divergence of quantum fluctuations of dynamical variables for classically chaotic trajectories in the early part of quantum evolution from a statistical mechanical point of view can thus be traced back in the correlation of the classical fluctuation. Our formulation is valid for N -degree-of-freedom systems and has been verified numerically on model Hamiltonian systems.

Keywords : Hamiltonian systems, Lyapunov exponents, Kubo relations, classical chaos

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1. Introduction

The mathematical development in the theory of nonlinear dynamics over the last few decades has provided great physical insight into our understanding of the nature of classical motion. The motion associated with the trajectories that remain confined to well-defined regions of phase space and show few changes in character when small changes in the initial conditions are made is termed regular. On the other hand, there are regimes in phase space where the trajectories are extremely sensitive to small changes in initial conditions and wander erratically over large regions of energetically accessible phase space. The motion of latter kind is unstable, irregular or chaotic. Over the last few decades the subject has seen phenomenal growth with considerable success in almost all areas of physics, chemistry and biology where nonlinearity prevails.

The extreme sensitivity to initial condition for nonlinear dynamical equations is quantitatively reflected in the positivity of the largest Lyapunov exponent which signifies an exponential separation of initially nearby trajectories. This, in turn, is associated with an enormous loss of initial correlations in the not-so-distant future such that the motion eventually

becomes as random as coin toss. For a certain class of systems known as C-systems this is a rigorous result. Although most Hamiltonian systems have not been proved to be C-systems, chaotic trajectories are found to display an exponential-like separation.

Thus although deterministic in principle, the chaotic motion is stochastic in nature. As a result one may easily comprehend a close connection between chaos and statistical mechanics. It is worthwhile to distinguish the two distinct situations in this context. The first one concerns whether chaotic motion can serve as a basis for statistical mechanics since the ultimate justification of the postulates of the statistical mechanics rests on the dynamics of each particle. With this end in view attempts have been made to justify Boltzmann's hypothesis of molecular chaos, ergodicity and the postulate of equal a priori probability from standpoint of loss of correlation of initially nearby trajectories of the particle comprising the macroscopic system. The second one on the other hand concerns the following : Given that a chaotic motion is truly stochastic, how and to what extent one can implement the statistical mechanical formalism for an useful description of classical chaos keeping in mind that one essentially deals here with a few-degree-of-freedom system. In this paper we address specifically the second issue.

To put the present issue in a proper prospective we first give a brief overview of some of the related recent developments. The statistical mechanical methods have been utilized in various ways in few-degree-of-freedom systems by a number of workers [1-7] in eighties. For example, Oono and Takahashi [2] have introduced a powerful method for characteristic multifractals based on certain partition functions. Widom *et. al.* [4] considered the example of Julia sets. The method of statistical physics was also followed by Kohmoto [5] to introduce the entropy and free energy functions for multifractals which are pre-requisite for the existence of thermodynamics. These functions are related to Kolmogorov-Sinai entropy and Lyapunov exponents in the case of dynamical systems. For continuous system the statistical mechanical method has been employed to define temperature and entropy analogous to thermodynamics.

Apart from equilibrium methods kinetic description [7-13] has also been utilized over the years. Ever since the early numerical study of Chirikov mapping [14] revealed that the motion of a phase space variable can be characterized by a simple random walk diffusion equation, attempts have been made to describe chaotic motion in terms of Langevin or Fokker-Planck equations. It has now been realized that deterministic maps can result in long time diffusional processes and methods have been developed to predict successfully the corresponding diffusion coefficients [15]. While these studies are based on maps, identification of a noise term in Lorenz equations after recasting it to an approximate Langevin form has been achieved by Nicolis and Nicolis [9] by successfully separating the distinct time-scales involved in the dynamics using a center manifold method. Bianucci *et. al.* [12] have considered a closed Hamiltonian system and showed that the system of interest follows a slower dynamics obeying a Fokker-Planck equation having a canonical distribution which defines a temperature-like quantity.

Since the emergence of stochasticity in a nonlinear dynamical system is essentially due to loss of correlation of two initially nearby trajectories, one can trace back its origin in the curvature (second derivative) of the potential in the Hamiltonian systems. When chaos has

fully set in, the time dependence of the curvature can be described as a stochastic process. In a number of recent studies [11, 16-17] we have shown that this fluctuation is amenable to a theoretical description in terms of the theory of multiplicative noise. This allows us to realize a number of important results of nonequilibrium statistical mechanics like Kubo relation, Fluctuation-dissipation relation, etc., in chaotic dynamics of few-degree-of-freedom systems. In this paper we discuss two such aspects ; first, the realization of Lyapunov exponent as a transport coefficient in Hamiltonian systems and second, identifying an early stage of quantum evolution of a classically chaotic system in terms of the exponential divergence of quantum fluctuations. The regime is dominated by chaotic diffusion. In presence of dissipation, the quantum system is governed by a Fokker-Planck equation reminiscent of Kramers' equation which describes the Brownian motion in phase space. The present stochastic approach reveals that the largest Lyapunov exponent as well as the rate of early exponential divergence of quantum fluctuations (or expansion in phase space) are determined by the correlation of fluctuations of the curvature of the classical potential, the key point being the chaotic diffusion in phase space. Our aim here is to employ the methods of stochastic differential equation for the description of this chaotic diffusion.

2. Curvature of the potential and stability of motion

Since the question of instability of nonlinear dynamical motion lies at the root of exponential separation of trajectories let us briefly recall the stability aspect which is relevant for our future discussions.

The classical equations of motion for a system with N degrees-of-freedom described by a Hamiltonian

$$H(p, q) = \frac{p \cdot p}{2} + U(q), \quad (1)$$

where p, q are N -dimensional vectors of momentum and conjugate coordinate respectively are given by

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -\nabla_q U(q). \end{aligned} \quad (2)$$

We now introduce the variables Δq and Δp , which measure the separation of the two trajectories in coordinate and momentum, respectively as

$$\begin{aligned} \Delta q(t) &= q^{(1)}(t) - q^{(2)}(t), \\ \Delta p(t) &= p^{(1)}(t) - p^{(2)}(t). \end{aligned} \quad (3)$$

For $q^{(2)}(t)$ sufficiently close to the reference trajectory $q^{(1)}$ one may obtain the linearized equations for Δq and Δp . Hence

$$\begin{aligned} \Delta \dot{q} &= \Delta p, \\ \Delta \dot{p} &= -V(t) \cdot \Delta q, \end{aligned} \quad (4)$$

where $\underline{V}(t)$ is the $N \times N$ matrix of the second derivative of the potential $U(\mathbf{q})$, evaluated along the reference trajectory. Thus

$$[\underline{V}(t)]_{ij} = \left[\frac{\partial^2 U(\mathbf{q})}{\partial q_i \partial q_j} \right]_{\mathbf{q}=\mathbf{q}^{(1)}(t)} \quad (5)$$

The stability of motion is determined by the time-dependent eigenvalues of $2N \times 2N$ matrix

$$\underline{M} = \begin{bmatrix} \underline{0} & \underline{1} \\ -\underline{V}(t) & \underline{0} \end{bmatrix}, \quad (6)$$

where $\underline{0}$ and $\underline{1}$ are the null and unit $N \times N$ matrices. The time dependent transformation \underline{S} diagonalises \underline{M} so that one has

$$[\underline{S}\underline{M}\underline{S}^{-1}]_{ij} = \lambda_i(t) \delta_{ij}. \quad (7)$$

If the real part of one of the eigenvalues is positive the trajectory separation grows exponentially and the motion becomes unstable.

Because of the inherent time-dependence, the eq. (7) is difficult to solve. As a primary step one, however, examines the stability around the equilibrium points determined by the condition $\dot{\mathbf{q}} = \dot{\mathbf{p}} = 0$, by freezing the time dependence of q -s in $\underline{V}(t)$. By minimizing the energy of a conservative system subject to the constraint of linear stability criteria it is possible to determine the stochasticity threshold. Such a contention was first proposed by Toda [18] and has been tested in Heiles-Henon and in a number of other related two-degree-of freedom systems by several workers [19].

While the above-mentioned stability analysis is local in nature, the true stability of motion is only determined by keeping the time-dependence of $\underline{V}(t)$ matrix intact. Also there is very little correlation between the local stability and global stochasticity. In view of this it is necessary to take full account of the time-dependence of the curvature of the potential $\underline{V}(t)$ along the reference trajectory itself. To this end we note the following two points.

First, when the motion of the dynamical system along the reference trajectory is regular $\underline{V}(t)$ is highly correlated throughout the entire course of evolution. On the other hand for a chaotic motion when the dynamical variables in $\underline{V}(t)$ behave stochastically, $\underline{V}(t)$ describes a stochastic process along the reference trajectory; the stochasticity originates from the chaotic motion itself. The loss of correlation in chaotic dynamical systems thus rests on the decay of correlation function of fluctuation of $\underline{V}(t)$, i.e., on $\langle \underline{V}(t) \underline{V}(t+\tau) \rangle$. What follows in the subsequent sections is a stochastic description of chaotic diffusion in phase space in terms of this correlation function in different physical situations. —

Secondly, although interpreted as a stochastic process, $\underline{V}(t)$ is determined dynamically from the numerical solution of classical equations of motion and as such one can not impose any a priori approximation on the nature of this stochastic process. The special cases that a stochastic process is Gaussian, or delta correlated, etc. have attracted so much attention in the literature that it is necessary to emphasize that we have not made any of such approximation on the nature of this stochastic process in the subsequent development of the present formulation.

3. Chaotic diffusion and instability of motion ; Kubo relations

Let us specialize the problem in the case of driven one-degree-of-freedom systems described by the following Hamiltonian

$$H = \frac{p^2}{2} + U(q) + gq \cos \omega t. \quad (8)$$

The first, second and the third terms represent the kinetic energy, potential energy and the driving term respectively. g and ω are the coupling constant and the frequency of the external field. $U(q)$ is assumed to be nonlinear such that nonlinearity renders the overall Hamiltonian nonintegrable. When full global chaos has set in one can treat q, p as stochastic variables.

The equation of motion and the equation of separation of trajectories are given by

$$\ddot{q} = -U'(q) - g \cos \omega t. \quad (9)$$

and

$$\ddot{\Delta q} = -U''(q) \Delta q. \quad (10)$$

The standard procedure [20] for calculation of the largest Lyapunov exponent (LLE), the positivity of which is an unambiguous measure of instability, is to solve the trajectory equation (9) and separation equation of motion (10) simultaneously for Δq and $\dot{\Delta q}$ as functions of time. The largest Lyapunov exponent is then given by

$$\lambda = \lim_{t \rightarrow \infty} \frac{\log \|d(t)\| / \|d(0)\|}{d(0) \rightarrow 0} \quad (11)$$

where the norm $\|d(t)\|$ is defined as

$$\|d(t)\| = [\dot{\Delta q}^2 + \Delta q^2]^{\frac{1}{2}}.$$

Since $U''(q)$ is, in general, a function of stochastic variable q , $U''(q)$ may be interpreted as a fluctuating quantity such that one may define fluctuation $\zeta(t)$ of $U''(q)$ as

$$\zeta(t) = U''(q) - U''(q_e^s), \quad (12)$$

where $U''(q_e^s)$ is the value of $U''(q)$ at one of the stable fixed points q_e^s determined by the condition $U'(q) = 0$. It is convenient to work with the following scaled quantities

$$\begin{aligned} \tau &= [U''(q_e^s)]^2 t \\ \tilde{U}'(q) &= U'(q) / U''(q_e^s) \\ \Omega &= \omega / [U''(q_e^s)]^{\frac{1}{2}} \\ \kappa &= g / U''(q_e^s) \end{aligned} \quad (13)$$

and express eqs. (9) and (10) in terms of them as

$$\frac{d^2 q}{d\tau^2} + \bar{U}'(q) = -\kappa \cos \Omega \tau \quad (14)$$

and

$$\frac{d^2 \Delta q}{d\tau^2} + \omega^2(\tau) \Delta q = 0, \quad (15)$$

where

$$\omega^2 = 1 + \alpha \zeta(\tau), \quad (16)$$

and

$$\alpha = [U''(q_e)]^{-1}.$$

Since $\zeta(\tau)$ is considered as a stochastic process, eq. (15) becomes an equation for harmonic oscillator with stochastic frequency $\omega^2(\tau)$.

We point out that we make no approximation about the nature of the stochastic process $\zeta(\tau)$, which is exactly determined by eq. (9) or (14).

The harmonic oscillator with random coefficients has been subject of extensive investigation over the last few decades, particularly in connection with wave propagation, line broadening, lasers, mechanical systems [21-23] *etc.* Eq (15) offers itself as a candidate for similar study in chaotic dynamics. What follows next we make use of a standard result derived by van Kampen [21] for linear stochastic differential equations. From eq. (15) one first derives

$$\frac{d}{d\tau} \begin{pmatrix} \Delta q^2 \\ \Delta \dot{q}^2 \\ \Delta q \Delta \dot{q} \end{pmatrix} = [A_0 + \alpha \zeta(\tau) B] \begin{pmatrix} \Delta q^2 \\ \Delta \dot{q}^2 \\ \Delta q \Delta \dot{q} \end{pmatrix}, \quad (17)$$

where A_0 and B are given by

$$A_0 = \begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & -2 \\ -1 & 1 & 0 \end{pmatrix}, \quad (18)$$

and

$$B = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2 \\ -1 & 0 & 0 \end{pmatrix}. \quad (19)$$

The equation of motion for the second moments are given by

$$\frac{d}{d\tau} \begin{pmatrix} \langle \Delta q^2 \rangle \\ \langle \Delta \dot{q}^2 \rangle \\ \langle \Delta q \Delta \dot{q} \rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 & 2 \\ \alpha^2 C_3 & -\alpha^2 C_2 & -2 - 2\alpha C \\ -1 - \alpha C + \alpha C_1 & 1 & -\alpha^2 C_2 \end{pmatrix} \begin{pmatrix} \langle \Delta q^2 \rangle \\ \langle \Delta \dot{q}^2 \rangle \\ \langle \Delta q \Delta \dot{q} \rangle \end{pmatrix} \quad (20)$$

where the average and the correlation functions of the fluctuation of the curvature of the potential are expressed as

$$\begin{aligned}
 C_1 &= \int_0^\infty \langle\langle \zeta(\tau) \zeta(\tau - \tau') \rangle\rangle \sin 2\tau \, d\tau', \\
 C_2 &= \int_0^\infty \langle\langle \zeta(\tau) \zeta(\tau - \tau') \rangle\rangle (1 - \cos 2\tau) \, d\tau', \\
 C_3 &= \int_0^\infty \langle\langle \zeta(\tau) \zeta(\tau - \tau') \rangle\rangle (1 + \cos 2\tau) \, d\tau', \quad | \\
 C &= \langle \zeta(t) \rangle, \\
 \langle\langle x_i x_j \rangle\rangle &= \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle.
 \end{aligned} \tag{21}$$

The relevant eigenvalue determined up to second order in α is

$$\lambda_0 = \alpha^2 (C_3 - C_2) \tag{22}$$

which corresponds to zero frequency of the unperturbed case [implying the conservation of $\frac{1}{2}(\Delta q^2 + \Delta p^2)$]. In the language of harmonic oscillator it is the energy which grows owing to the fluctuation in the force that have twice the proper frequency of the oscillator. Or in other words the separation of the nearby trajectories grows exponentially at a rate λ_0 . So when expressed in terms of relations (21) the L L E is given by

$$\lambda = \frac{\alpha^2}{2} \int_0^\infty \langle\langle \zeta(\tau) \zeta(\tau - \tau') \rangle\rangle \cos 2\tau \, d\tau'. \tag{23}$$

The above result associates the L L E to the correlation function of fluctuations of the curvature of the potential. Since the divergence of separation of the trajectories is responsible for diffusive motion in phase space, the relation (23) may be viewed as a fluctuation-diffusion relation in chaotic dynamics. Secondly, the formal similarity of eq. (23) with Kubo relation for transport co-efficients, such as, conductivity σ expressed as a Fourier transform of current-correlation function as

$$\sigma(\omega) = \frac{1}{kT} \int_0^\infty \exp(-i\omega\tau) \langle J(0) J(\tau) \rangle d\tau, \tag{24}$$

can hardly be overlooked. Thus eq. (23) can alternatively be viewed as a Kubo relation in chaotic dynamics and L L E as a transport coefficient for Hamiltonian systems. Detailed numerical calculation for the specific choice of the $U(q)$ ensures that the agreement between the above theoretical proposition and the L L E calculated by the standard method of Benettin *et. al.* [20] is fairly satisfactory. The theory can also be generalized to treat N-degree of freedom Hamiltonian systems.

A few [11] related parallel as well as subsequent developments may be noted here. Evans [24] has derived a fluctuation expression for the temperature derivative of the L L E for a large system in contact with a thermal bath. The resulting equation is similar to statistical mechanical expression for temperature derivatives of thermodynamic variables in a canonical ensemble. Suhl [25] has discussed chaos in the context of a Kubo formula. Barnett and Tajima

[26] have established a link between Lyapunov exponents, correlation functions and transport coefficients in a many-body system. Stochastic perturbation theory has been used to derive a proportional relationship between the L L E of a many-body system and the correlation function of the second derivative of the interparticle potential. Two specific cases have been examined by them ; (i) a weakly coupled gas and (ii) one dimensional mono-atomic lattice with nonlinear nearest neighbour coupling. They have shown that the connection with transport coefficients can also be established in a many-body system.

4. Chaotic diffusion and quantum evolution

In the last section, we have discussed the role of fluctuation of the curvature of the potential in determining the global stability of motion and how the instability results in chaotic diffusion in phase space. We now address ourselves to the question of quantum evolution. In this context, we first point out an interesting observation of some numerical experiments carried out recently [16 and 27-28] in a number of prototype Hamiltonian systems. It was demonstrated that the initial growth of quantum fluctuations of the canonical dynamical variables, such as, position or momentum for a classically chaotic trajectory is exponential in nature. This has been identified as a semiclassical manifestation of classical chaos. In this section, we focus our attention on this aspect, particularly to examine the evolution of quantum fluctuations. The present analysis reveals that the rate of early exponential growth depends crucially on the correlation of classical fluctuations of the curvature of the potential. When dissipation is incorporated in the system we show that an interplay of chaotic diffusion and dissipation leads to an ultimate equilibrium in the dissipative systems. We make use of Wigner's distribution function [29] and \hbar -scaling [27] in our semiclassical analysis and derive appropriate Fokker-Planck equation, where the drift and diffusion terms have their origin in the dynamical properties of classical chaos and dissipation due to an external thermal bath.

To start with, we consider a quantum system in contact with a thermal bath. The Hamiltonian of an N-degree-of-freedom system is given by

$$H_0 = \sum_{i=1}^N \frac{p_i^2}{2m_i} + U(\{q_i\}), \quad i = 1 \dots N, \quad (25)$$

where $\{q_i, p_i\}$ represents the coordinates and momenta of the system.

The bare system is now coupled to a reservoir of harmonic oscillator modes. After appropriate elimination of reservoir variables in the usual way, using Born and Markov approximations we are led to the following reduced density matrix equation for the evolution of the system [30-31]

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H_0, \rho] + \frac{\gamma}{2} (2a\rho a^\dagger - a^\dagger a \rho - \rho a^\dagger a) + D(a^\dagger \rho a + a \rho a^\dagger - a^\dagger a \rho - \rho a a^\dagger). \quad (26)$$

Here a and a^\dagger are annihilation and creation operators. We have assumed that only one (q) of the system modes is coupled to reservoir, where $q = \frac{1}{\sqrt{2m\omega}} (a + a^\dagger)$. ω refers to the frequency of the harmonic oscillator on the basis of which full quantum calculations are performed. γ is the relaxation or dissipation rate and $D (= \bar{n} \gamma)$ is the thermal diffusion coefficient. $\bar{n} (= [\exp(\frac{\hbar\omega}{kT}) - 1]^{-1})$ is the average thermal photon number of the reservoir.

The first term in eq. (26) corresponds to the dynamical motion of the system that generates Liouville flow. The second term implies the loss of energy from the system to the reservoir, while the last term indicates the diffusion of fluctuations of the reservoir modes into the system of interest. The terms containing γ arise due to the interaction with the surroundings.

Eq. (26) is the basic starting point of our analysis. Our next task is to transform the full quantum problem to an equivalent c -number problem described by the Hamiltonian which leads to Eq. (26). A standard procedure is to apply Wigner distribution function W [29, 34] and the time evolution of the dynamical system is now given by,

$$\begin{aligned} \frac{\partial W}{\partial t} = & \sum_{i=1}^N \left[-\frac{p_i}{2m_i} \frac{\partial W}{\partial q_i} + \left(\frac{\partial U}{\partial q_i} \right) \frac{\partial W}{\partial p_i} \right] \\ & + \sum_{\substack{n_1 + \dots + n_N \\ \text{odd and } > 1}} \left(\frac{\partial^{n_1 + \dots + n_N} U}{\partial^{n_1} q_1 \dots \partial^{n_N} q_N} \right) \frac{\left(\frac{\hbar}{2i} \right)^{n_1 + \dots + n_N - 1}}{n_1! \dots n_N!} \\ & \times \frac{\partial^{n_1 + \dots + n_N}}{\partial^{n_1} p_1 \dots \partial^{n_N} p_N} W + 2\gamma \frac{\partial}{\partial p} p W + D \frac{\partial^2 W}{\partial p^2} \end{aligned} \quad (27)$$

The first term is the usual Poisson bracket which generates classical motion. Both the Poisson bracket and the higher derivative terms result from an expansion of the Moyal bracket on the basis of an analytic $U(q)$. The last two terms are the same as those of eq. (26) but without the rotating wave approximation. It is important to note that the failure of correspondence between classical and quantum dynamics is predominantly due to higher derivative terms [29] which make their presence felt roughly beyond the Erhenfest regime.

As a first step we invoke the symplectic structure of the Hamiltonian dynamics. For this, we specify

$$z_i = \begin{cases} q_i & \text{for } i = 1 \dots N \\ p_{i-N} & \text{for } i = N + 1, \dots 2N. \end{cases} \quad (28)$$

Defining I as

$$I = \begin{pmatrix} 0 & E \\ -E & 0 \end{pmatrix}, \quad (29)$$

where E is an $N \times N$ unit matrix, one can write the Hamilton's equation

$$\dot{z}_i = \sum_j I_{ij} \frac{\partial H}{\partial z_j} \quad (30)$$

In the second step, we introduce the scaling z_i in analogy to van Kampen's Ω -expansion as [16 and 27]

$$z_i = z_i(t) + \hbar^{1/2} \eta_i \quad (31)$$

with

$$\begin{aligned}\eta_i &= \mu_i & \text{for } i = 1, \dots, N \\ &= v_{i-N} & \text{for } i = N+1, \dots, 2N\end{aligned}\quad (32)$$

η -s refer to quantum fluctuation variables in coordinate (μ_i) and momentum (v_i). One obtains the equation of motion for quantum fluctuation distribution function.

$$\frac{\partial \phi(\eta)}{\partial t} = - \sum_{i,j} \left[J_{ij} \eta_i \frac{\partial \phi(\eta)}{\partial \eta_j} - 2\gamma \frac{\partial}{\partial \eta_j} (\eta_j \phi(\eta)) \right] \quad (33)$$

where we have assumed that $\gamma_j = 0$ for $j = 1, \dots, N$

and $\gamma_j = \nu$ for $j = N+1, \dots, 2N$

Here

$$J_{ij} = \sum_k I_{ik} \frac{\partial^2 H}{\partial z_i \partial z_k} \quad (34)$$

contains the second derivatives of the potential. The matrix \underline{J} is thus determined by the nature of the classical motion. For chaotic motion, the stochastic fluctuations of \underline{J} thus affect the evolution of quantum fluctuations as determined by eq. (33).

For further treatment eq. (33) may be rewritten in a more compact form as follows :

$$\frac{\partial \phi}{\partial t} = [-\underline{F}(t) \cdot \nabla + 2N\gamma] \phi, \quad (35)$$

where

$$\underline{F}(t) = \underline{J}(t) \underline{\eta} - 2\gamma \underline{K} \underline{\eta}. \quad (36)$$

∇ refers to differentiation with respect to components of $\underline{\eta}$. \underline{K} is a $2N \times 2N$ matrix defined as

$$\begin{aligned}K_{ij} &= 0 & i \neq j \\ K_{ii} &= 0 & \text{for } i = 1, \dots, N \\ K_{ii} &= 1 & \text{for } i = N+1, \dots, 2N\end{aligned}$$

Two important points are to be noted here. First, we consider a *fully developed strong chaos* such that the measure of regular region is sufficiently small so that $\underline{F}(t)$ in eq. (35), which is governed by classical chaotic fluctuations in the curvature of the potential [eq. (34)] can be treated as a stochastic process.

Second, we do not make any *a priori* assumption about the nature of the stochastic process $\underline{F}(t)$. Eq. (35) may therefore be regarded as a stochastic differential equation with multiplicative noise. We note that $\underline{F}(t) \cdot \nabla$ can be partitioned into two parts ; a constant part $\underline{F}_0 \cdot \nabla$ and a fluctuating part $\underline{F}_1(t) \cdot \nabla$. Thus we write.

$$\underline{F} \cdot \nabla = \underline{F}_0 \cdot \nabla + \underline{F}_1 \cdot \nabla. \quad (37)$$

We now proceed to the third step. Making use of one of the main results for the theory of linear equation of the form eq. (35) with multiplicative noise, we derive an average equation for ϕ as given by (for details, we refer to [21]) ;

$$\frac{\partial \langle \phi \rangle}{\partial t} = \left\{ -F_0 \cdot \nabla + 2N\gamma - \langle F_1 \cdot \nabla \rangle + \int_0^\infty d\tau \left| \frac{d\eta^{-\tau}}{d\eta} \right| \right. \\ \left. \left\langle \left\langle F_1(\eta, t) \cdot \nabla_\tau F_1(\eta^{-\tau}, t-\tau) \right\rangle \right\rangle \cdot \nabla_{-\tau} \left| \frac{d\eta}{d\eta^{-\tau}} \right| \right\} \langle \phi \rangle. \quad (38)$$

The above consideration is based on an expansion in $\alpha\tau_c$ (by van Kampen), where α is the strength and τ_c is the correlation time of fluctuations [in the derivation above we have put $\alpha = 1$]. The expansion is valid in the case where fluctuations are not too large but rapid and correlation time τ_c is short but finite. Second, the derivation above neglects the effects of higher powers of \hbar and thus the eq. (38) is an effective semiclassical equation for quantum fluctuation distribution function. Since it contains second derivatives with respect to components of $\bar{\eta}$, it has the form of a Fokker-Planck equation. Third, the theory discussed so far is valid, in general, for N-degree-of-freedom chaotic systems in presence of dissipation.

We now return to the specific one-degree-of-freedom Hamiltonian system [eq. (8)] for illustration of general eq. (38). For this purpose we choose $U(q) = aq^4 - bq^2$. Note that $N = 1$.

The equations of motion for quantum fluctuation variables η_1 and η_2 corresponding to q and p read as follows :

$$\frac{d}{dt} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \underline{J} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} \quad (39)$$

Following the procedure as described earlier \underline{J} can be calculated as

$$\underline{J} = \begin{pmatrix} 0 & \frac{1}{m} \\ -U''(q) & 0 \end{pmatrix}. \quad (40)$$

with $-U''(q) = \zeta(t) + 2b$, where $\zeta(t)$ and $2b$, represent the fluctuating and the constant parts of the curvature of the potential $U(q)$, respectively. Here $\zeta(t)$ is given by

$$\zeta(t) = -12aq^2.$$

If one takes into consideration of the γ -term then $\mathbf{F}(t)$ in eq. (36) can be identified as

$$\mathbf{F} = \mathbf{F}_0 + \mathbf{F}_1(t), \quad (41)$$

where

$$\mathbf{F}_0 = \begin{pmatrix} \frac{1}{m}\eta_2 \\ 2b\eta_1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & -\gamma \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} \\ = \begin{pmatrix} \frac{1}{m}\eta_2 \\ 2b\eta_1 - \gamma\eta_2 \end{pmatrix} \quad (42)$$

and

$$\mathbf{F}_1(t) = \begin{pmatrix} 0 \\ \zeta(t)\eta_1 \end{pmatrix} \quad (43)$$

Making use of the mapping transformations $\eta \rightarrow \eta^\tau$ for the unperturbed motion one calculates the first and second derivative terms in eq. (38) [For details we refer to [21]]. The Fokker-Planck equation can then be written in a compact form as follows :

$$\frac{\partial \langle \phi \rangle}{\partial t} = -\frac{\eta_2}{m} \frac{\partial \langle \phi \rangle}{\partial \eta_1} - \omega'^2 \eta_1 \frac{\partial \langle \phi \rangle}{\partial \eta_2} + \gamma \frac{\partial}{\partial \eta_2} (\eta_2 \langle \phi \rangle) + A' \frac{\partial^2 \langle \phi \rangle}{\partial \eta_2^2} + B \frac{\partial^2 \langle \phi \rangle}{\partial \eta_1 \partial \eta_2} \quad (44)$$

where

$$\begin{aligned} c &= \langle \zeta(t) \rangle, \\ c_1 &= \int_0^\infty \langle \zeta(t) \zeta(t-\tau) \rangle e^{-\gamma \tau} d\tau, \\ c_2 &= \int_0^\infty \langle \zeta(t) \zeta(t-\tau) \rangle e^{-\gamma \tau} \tau d\tau, \\ A' &= \eta_1^2(0) c_1 - \eta_1(0) \eta_2(0) c_2, \\ B &= \eta_1^2(0) c_2, \\ \omega'^2 &= 2b + c + c_2, \\ m &= 1. \end{aligned} \quad (45)$$

Note that in the expressions for diffusion coefficients A' and B we have frozen the time-dependence of η_1 and η_2 by setting their initial values. This corresponds to the weak noise approximation. The above Fokker-Planck equation which governs the evolution of distribution of quantum fluctuations η_1 and η_2 corresponding to co-ordinate and momentum variables, respectively, in presence of dissipation has a formal similarity in structure to Kramers' equation [32] which describes the Brownian motion of a particle in phase space. While the stochasticity in Kramers' equation originates from the thermal fluctuations derived from the true statistical properties of the reservoir which is a many body system, the stochasticity in the present problem owes its origin to the dynamical properties of classical chaos in a low dimensional system.

We now take into account of appropriate quantum-classical correspondence by searching a conditional probability solution for $\langle \phi(\eta, t) \rangle$ subject to an initial condition which corresponds to a coherent state. The uncertainty in coordinate $\Delta\eta_1$ and that in momentum $\Delta\eta_2$ are then given by :

$$\begin{aligned} \Delta\eta_1^2 &= \langle \eta_1^2 \rangle - \langle \eta_1 \rangle^2 = \frac{1}{\omega} \left[\frac{\Gamma(t)}{2} \right], \\ \Delta\eta_2^2 &= \langle \eta_2^2 \rangle - \langle \eta_2 \rangle^2 = \left[\frac{\Gamma(t)}{2} \right] \omega. \end{aligned} \quad (46)$$

The uncertainty product $\Delta\eta_1 \Delta\eta_2$ at any time is then given by

$$\Delta\eta_1 \Delta\eta_2 = \frac{1}{2} \Gamma(t), \quad (47)$$

where $\Gamma(t)$ is expressed as

$$\Gamma(t) = \Gamma(0) e^{-\gamma t} + \frac{2A}{\gamma} (1 - e^{-\gamma t}), \quad (48)$$

with

$$A = \frac{A'}{\omega}, \quad \Gamma(0) = 1. \quad (49)$$

The eqs. (46-47) relate the evolution of quantum fluctuations as functions of time in terms of $\Gamma(t)$ which by the virtue of eq. (49) is determined by the initial condition $\Gamma(0)$ and the other two parameters A and γ . Note that A is the diffusion coefficient defined by eqs. (45) and 49) [this is not to be confused with the thermal diffusion coefficient D in eq. (26) which arises due to the interaction with the surroundings] and γ refers to the dissipation rate of the system in contact with the surroundings. Since A is related to the fluctuations of the curvature of the classical potential $\zeta(t)$ through c_2 and c_1 in eq. (45), the origin of diffusion coefficient A is essentially the classical chaos.

To analysis the growth of quantum fluctuations quantitatively [eq. 47] we now consider the classical chaotic motion governed by the Hamiltonian (25) and introduce a phenomenological damping γ in the classical equation of motion. We choose the parameter values $m = 1$, $a = 0.5$, $h = 10$, $\omega_0 = 6.07$, $\gamma = 0.001$. The coupling constant cum field strength, g is choosen 14.0 and 18.0 for two sets when other parameters remain fixed. We also choose the initial condition $q_0 = -3.5$ and $p_0 = 0.0$, which ensures strong global chaos. To calculate classical ensemble average of the quantities like $\langle \zeta(t) \rangle$ and $\langle \langle \zeta(t) \zeta(t - \tau) \rangle \rangle$ which appeared in the expression for chaotic diffusion coefficient A in eqs. (45 and 48), we carry out averaging over long time series.

For a full quantum-mechanical calculation to verify the basic theoretical propositions of semiclassical dynamics [eq 47] we now return to eq. (26). The eigenvectors $|n\rangle$ of a harmonic oscillator which satisfies $[(\hat{p}^2 / 2m + (1/2)m\omega^2 \hat{q}^2)]|n\rangle = [(n + 1/2) \hbar \omega]|n\rangle$ are chosen as basis vectors to solve eq. (26). The frequency ω is arbitrarily adjusted to economize the size of the basis set. For the present purpose, we choose $\omega = 6.25$, $\hbar = 1$, and 120 basis vectors. In this representation, the equations of motion for the reduced density matrix elements (eq. 26) are solved. The quantum evolution is followed by locating the average position and average momentum of the initial coherent wave packet corresponding to the initial position and momentum of a classically chaotic trajectory. As a numerical check we have compared our results with those of Lin and Ballentine [33] in classical and quantum cases for $D = 0$, $\gamma = 0$. Another important check for the numerical calculation is the keep $\text{Tr} \rho = 1$ for the entire evolution.

Having calculated A as described above we follow eq. (47) to plot a typical representative variation of $\ln [\Delta \eta_1 \Delta \eta_2]$ ($\Delta \eta_1$ and $\Delta \eta_2$ are the quantum variances corresponding to position and momentum, respectively) as a function of time in Figures 1 (a, b) (dotted line) for different values of g . This is compared with full quantum calculation for the above-mentioned parameter values (full line). We have also checked basic proposition for other parameter sets. The agreement is found to be quite satisfactory in all cases.

We summarize the main results of this section.

(i) \hbar -scaling identifies an early stage of quantum evolution in which the thermal diffusion term has no significant part to play.

(ii) This stage is dominated by chaotic diffusion. The drift and diffusion terms have their origin in the intrinsic dynamical properties of the classical chaotic system. Formally, the Fokker-Planck equation is identical in structure with Kramers' equation which describes a Brownian dynamics in phase space and is valid for general N -degree-of-freedom Hamiltonian systems.

(iii) We have analytically solved this equation as an initial value problem to study the evolution of quantum variances for a specific example. It can also be shown that the dissipation plays a significant role for attainment of equilibrium.

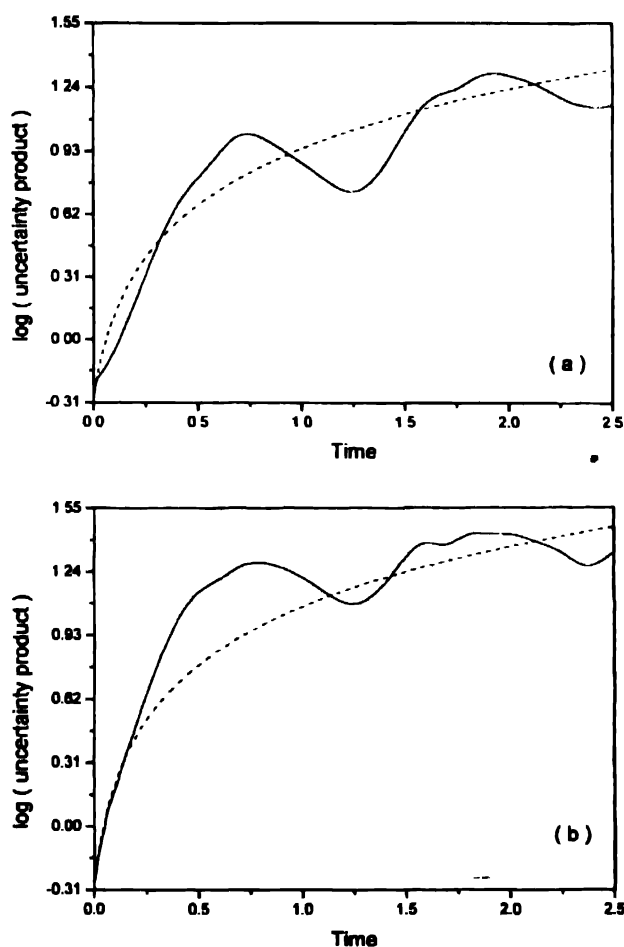


Figure 1 : Plot of log of uncertainty product with time for different values of g . The continuous line represents the numerical calculation (fully quantum). The dotted line refers to semiclassical calculation (eq. (24)). (a) $g = 14.0$ and (b) $g = 18.0$. (Both units are arbitrary).

5. Conclusions

A key-point in determining the stability of motion in a nonlinear dynamical system rests on the fluctuation of the curvature of the potential. We have shown that this fluctuation is amenable to an analysis in terms of a theory of multiplicative noise. We take full account of the noise process generated by exact solution of the classical equations of motion and as such no explicit or implicit assumption on the nature of this process is made in the treatment. The validity of the theory, however, lies on the shortness (but finite) of the correlation time compared to the coarse-grained timescale over which the average dynamics evolves in time. We also note that, however small the fluctuation is, this leads to exponential separation of initially nearby trajectories. Thus the fluctuation of curvature of the potential may be identified as a generic cause of instability of classical motion. We have also shown that the correlation of fluctuation of the potential is instrumental in determining the early rate of divergence of quantum fluctuations. Furthermore in a dissipative system the interplay of dissipation and chaotic diffusion results in a situation which mimics the conventional Brownian motion in phase space, described by Kramers' equation. Although chaos implies stochasticity in low-dimensional system our theoretical propositions on the Kubo relations and analogy to Kramers' equation carry the message that deterministic strong chaos can be conveniently described within the framework of time-correlation function methods and nonequilibrium statistical mechanics, in general.

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